

# PT Symmetry in Classical and Quantum Statistical Mechanics

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## Abstract

$\mathcal{PT}$ -symmetric Hamiltonians and transfer matrices arise naturally in statistical mechanics. These classical and quantum models often require the use of complex or negative weights and thus fall outside of the conventional equilibrium statistical mechanics of Hermitian systems.  $\mathcal{PT}$ -symmetric models form a natural class where the partition function is necessarily real, but not necessarily positive. The correlation functions of these models display a much richer set of behaviors than Hermitian systems, displaying sinusoidally-modulated exponential decay, as in a dense fluid, or even sinusoidal modulation without decay. Classical spin models with  $\mathcal{PT}$  symmetry include  $Z(N)$  models with a complex magnetic field, the chiral Potts model and the anisotropic next-nearest-neighbor Ising (ANNNI) model. Quantum many-body problems with a non-zero chemical potential have a natural  $\mathcal{PT}$ -symmetric representation related to the sign problem. Two-dimensional QCD with heavy quarks at non-zero chemical potential can be solved by diagonalizing an appropriate  $\mathcal{PT}$ -symmetric Hamiltonian.

## I. INTRODUCTION

The fundamental importance of  $\mathcal{PT}$  symmetry was first pointed out by Bender and Boettcher in their seminal work on quantum-mechanical models [6]. Their work grew out of the observation that the Hamiltonian

$$H = p^2 + igx^3. \quad (1)$$

has only real eigenvalues. Bender and Boettcher observed that the Hamiltonian  $H$ , while not Hermitian, is invariant under the simultaneous application of the symmetry operations parity  $\mathcal{P} : x \rightarrow -x$  and time reversal  $\mathcal{T} : i \rightarrow -i$ . This symmetry ensures that all eigenvalues of  $H$  are either real or part of a complex pair. The argument is simple: if  $H|\psi\rangle = E|\psi\rangle$  then  $H\mathcal{PT}|\psi\rangle = \mathcal{PT}H|\psi\rangle = \mathcal{PT}E|\psi\rangle = E^*\mathcal{PT}|\psi\rangle$ . Thus if  $E$  is an eigenvalue,  $E^*$  is an eigenvalue as well. The unexpected feature of the  $ix^3$  model discovered by Bender and Boettcher is that all of its eigenvalues are real. Since that discovery, research on  $\mathcal{PT}$ -symmetric systems has grown enormously, with applications in many areas of physics [4, 5].

The  $ix^3$  model has its origins in the study of the Lee-Yang theory of phase transitions [27, 43]. Lee and Yang showed how the critical properties of the Ising model could be studied using an analytic continuation of the external magnetic field  $h$  to imaginary values. They demonstrated that the zeros of the partition function were all on the line  $\text{Re}(h) = 0$ , reaching the real axis at the critical point. It was subsequently realized that the phase transition the edge of the gap in the distribution of zeros above the critical temperature is itself a critical point described by an  $i\phi^3$  field theory [20]. In two dimensions, this field theory at its critical point yields the simplest of the non-unitary minimal conformal field theories [12, 13, 44, 45]. In one dimension, the  $i\phi^3$  field theory reduces to  $ix^3$  quantum mechanics. There is a connection between  $\mathcal{PT}$ -symmetric quantum mechanical models and conformal field theories in two dimensions [19]. This connection is closely related to the proof that a large class of  $\mathcal{PT}$ -symmetric quantum mechanical models, including the  $ix^3$  model, have only real spectra [17]; see also [18].

Our focus here will be the application of generalized  $\mathcal{PT}$  symmetry to some well-known models of statistical mechanics. By generalized  $\mathcal{PT}$  symmetry, we mean that the relevant unitary operator is not necessarily the parity operator; in many cases, the role of  $\mathcal{P}$  will be played by the charge conjugation operator. Some models, such as the  $Z(N)$  spin model with

a complex magnetic field, will have a direct connection to Lee-Yang theory. In other cases, such as the anisotropic next-nearest-neighbor Ising model (ANNNI model) [39] or the chiral Potts model [24, 36], no complex numbers will appear in the formulation of the model and the appearance of  $\mathcal{PT}$  symmetry will be hidden.

For those already familiar with the subject of  $\mathcal{PT}$  symmetry, we should emphasize that the focus here is somewhat different from the majority of work on the subject. We are interested in extant models in statistical mechanics in which  $\mathcal{PT}$  symmetry plays a role, and not on the statistical mechanics of  $\mathcal{PT}$ -symmetric models *per se*. There are some differences between the application of  $\mathcal{PT}$  symmetry to statistical mechanics and work on  $\mathcal{PT}$ -symmetric quantum mechanics. For the models we discuss, the question of integration contours in the complex plane does not arise. Furthermore, the standard inner product, as opposed to the CPT inner product often used in  $\mathcal{PT}$ -symmetric quantum mechanics, is sufficient. Thus the models we discuss are similar to the Ising model in an imaginary field, which is the prototypical example of  $\mathcal{PT}$  symmetry in statistical mechanics.

Our original interest in this subject was motivated by the sign problem, particularly its appearance in QCD at finite density [29, 40]. Essentially, the sign problem is really an instance of the general problem of complex weights in a statistical sum. Such weights may arise because the Hamiltonian or action is complex; as we explain below, the problem arises naturally in Euclidean quantum field theories with non-zero chemical potential. The sign problem is a large barrier to first-principles lattice simulations of QCD at finite density and the study of color superconductivity [1]. As we show in section V, all Euclidean quantum field theories with a sign problem due to a non-zero chemical potential have a generalized  $\mathcal{PT}$  symmetry. The class of statistical models with generalized  $\mathcal{PT}$  symmetry is very large. We will show below that this class is precisely the set of models for which the complex weight problem can be reduced to a sign problem, *i.e.*, there is a representation in which the partition function is constructed from only real, but not necessarily positive, weights. We believe that generalized  $\mathcal{PT}$  symmetry is likely to play a role in any future solution of the sign problem.

The spectral properties of statistical models with  $\mathcal{PT}$  symmetry are different from those of Hermitian theories, which have the property of spectral positivity. Essentially, this property ensures that connected two-point correlation functions of observable will fall monotonically to zero with separation. When there is a mass gap between the ground state and the lowest

excited state, this mass gap determines a minimum rate of exponential decay for correlation functions. Systems with generalized  $\mathcal{PT}$  symmetry need not have spectral positivity, and their two-point correlation functions can show sinusoidally-modulated exponential decay, as in a dense fluid, or even sinusoidal modulation without decay, as in periodic phases. Because these behaviors are observed in nature, it is perhaps unsurprising that  $PT$  symmetry occurs in many problems of statistical mechanics.

The remainder of this article is structured as follows: section II introduces the fundamentals of generalized  $\mathcal{PT}$  symmetry and its role in the sign problem. Section III discusses the general spectral properties of  $\mathcal{PT}$ -symmetric models. In section IV, we treat several models from classical statistical mechanics. Section V consider quantum statistical models. We show how  $\mathcal{PT}$  symmetry makes it possible to solve a form of two-dimensional QCD at finite density. A final section provides brief concluding remarks.

## II. FUNDAMENTALS OF $\mathcal{PT}$ SYMMETRY AND THE SIGN PROBLEM

In this section, we discuss some fundamental aspects of  $\mathcal{PT}$  symmetry. We also discuss here some fundamental aspects of the sign problem that have a close relation with  $\mathcal{PT}$  symmetry. Although we will for the most part consider  $\mathcal{PT}$ -symmetric Hamiltonians, in classical statistical mechanics it is often most natural to work with  $\mathcal{PT}$ -symmetric transfer matrices, and the results for Hamiltonians have obvious counterparts for transfer matrices. Typically, the transfer matrix  $T$  of a lattice model acts as a Euclidean propagator similar to  $\exp(-tH)$  in a particular lattice direction. If the lattice has length  $L$  in that direction, then with periodic boundary conditions the partition function is  $Z = \text{Tr}(T^L)$ . It is sometimes convenient to identify  $L$  with  $\beta$  and  $T$  with  $\exp(-H)$  so that  $\text{Tr}(T^L)$  can be written as  $\text{Tr}(\exp(-\beta H))$ .

### A. Eigenvalues of $\mathcal{PT}$ -symmetric systems

Given a Hilbert space, the adjoint  $H^+$  of an operator  $H$  is defined using the inner product:

$$\langle \phi | H^+ | \psi \rangle = \langle \psi | H | \phi \rangle^* \quad (2)$$

which we often write as

$$H^+ = H^{*T}. \quad (3)$$

Operators satisfying  $H^\dagger = H$  are said to be Hermitian (we follow the usual physics practice and do not distinguish between Hermitian and self-adjoint operators). It is a standard result that the eigenvalues of a Hermitian operator are real. Operators with a generalized  $\mathcal{PT}$  symmetry have a more general constraint on their eigenvalues: they are either real or form a complex conjugate pair. A Hamiltonian  $H$  is  $\mathcal{PT}$ -symmetric if  $[H, \mathcal{PT}] = 0$ . Let  $|\psi\rangle$  be an eigenstate of  $H$  with eigenvalue  $E$ . Then we have  $H\mathcal{PT}|\psi\rangle = \mathcal{PT}H|\psi\rangle = \mathcal{PT}E|\psi\rangle = E^*\mathcal{PT}|\psi\rangle$ . Thus we see that  $\mathcal{PT}|\psi\rangle$  is an eigenstate of  $H$  with eigenvalue  $E^*$ . If  $|\psi\rangle$  is an eigenstate of  $\mathcal{PT}$ , then necessarily  $E$  is real. However,  $\mathcal{PT}$ -symmetric Hamiltonians can also have complex conjugate pairs of eigenvalues. The case where two or more eigenvalues are not real is usually described as broken  $\mathcal{PT}$  symmetry. Eigenstates of  $H$  associated with a complex eigenvalue pair cannot be eigenstates of  $\mathcal{PT}$ . In the models we consider,  $\mathcal{T}$  is implemented as complex conjugation, and  $\mathcal{P}$  is a unitary operator obeying  $[\mathcal{P}, \mathcal{T}] = 0$  and  $\mathcal{P}^2 = 1$ .

## B. Bender-Mannheim theorem

Not all  $\mathcal{PT}$ -symmetric models are obviously so. A simple criterion for a  $\mathcal{PT}$ -symmetric Hamiltonian  $H$  (or transfer matrix  $T$ ) has been given by Bender and Mannheim [10]. If the characteristic polynomial  $\det[H - \lambda I]$  has real coefficients, then  $H$  has a generalized  $\mathcal{PT}$  symmetry. Interesting models arise in statistical mechanics with hidden  $\mathcal{PT}$  symmetry when the transfer matrix  $T$  is real but not symmetric, as will be discussed below in section IV.

The striking feature of the  $ix^3$  models is that all of its energy eigenvalues are real. This is usually referred to as unbroken  $\mathcal{PT}$  symmetry. We will distinguish three different behaviors of  $\mathcal{PT}$ -symmetric models, based on the reality of the eigenvalues of the Hamiltonian  $H$  or transfer matrix  $T$ . We order the eigenvalues of  $H$  by their real parts, so that the ground state of  $H$  has the eigenvalue with the lowest real part. Similarly, we order the eigenvalues of  $T$  by their magnitude; the eigenvalue largest in magnitude is the analog of the ground state energy. Typically the different behaviors are each associated with a different part of parameter space. In region I,  $\mathcal{PT}$  symmetry is unbroken, and all eigenvalues are real. In region II, the lowest eigenvalue of  $H$  is real, but  $\mathcal{PT}$  symmetry is broken by one or more pairs of excited states becoming complex. For a transfer matrix  $T$ , the eigenvalue largest in absolute value is real

in region II, but other eigenvalues are complex. In region III,  $\mathcal{PT}$  symmetry is broken by the ground state of  $H$  becoming complex. For a transfer matrix  $T$ , the eigenvalue of largest absolute value becomes complex. Strictly speaking, by our definition above this means there are two ground states. This does not occur in conventional quantum-mechanical systems with a finite number of degrees of freedom, but does occur in  $\mathcal{PT}$ -symmetric models. It also occurs, of course, in Hermitian models with an infinite number of degrees of freedom, and is the basis of spontaneous symmetry breaking. As we show in the next section, this distinction is physical, and manifests directly in correlation functions. In region II, oscillatory behaviors appears in correlation functions. In region III, the system is in a spatially modulated phase. We emphasize that the behavior of correlation functions seen in regions II and III cannot be obtained from conventional models for which  $H$  is Hermitian: such behavior is incompatible with the spectral representation of the correlation function for Hermitian theories.

### C. Connection to complex weight problem

A naive treatment of  $\mathcal{PT}$ -symmetric models often involves a sum over complex weights, as in the path integral treatment of the  $ix^3$  model or in the continuation of the Ising model to imaginary magnetic field. In many areas of physics, there are problems where we wish to evaluate the “average” of some quantity  $x$  over an ensemble with complex weights  $w_j \in \mathbb{C}$  :

$$\langle x \rangle \equiv \frac{\sum_j x_j w_j}{\sum_j w_j} \quad (4)$$

There is no effective general algorithm for calculating such sums, as is the case for positive weights; see, *e.g.*, [14, 15, 28]. This problem is generally referred to as the sign problem, because even the case of negative weights is difficult. We will discuss the sign problem in detail for several models in sections IV and V, but here discuss the general role of  $\mathcal{PT}$  symmetry. Let us consider the case where the  $w_j$ ’s can be written as  $\exp(-\beta E_j)$ , as is typical in statistical mechanics where  $E_j$  is eigenvalue of some operator  $H$  and  $\beta$  is the inverse of the temperature  $T$ . For a Hermitian system, the partition function

$$Z(\beta) = \sum_j e^{-\beta E_j} \quad (5)$$

is real and positive for all real values of  $\beta$ , because the eigenvalues are all real. On the other hand, if  $H$  is  $\mathcal{PT}$ -symmetric, the eigenvalues are either real or occur in complex conjugate

pairs. We will prove in sections III that  $Z$  may be represented as

$$Z(\beta) = \sum_{\text{real}} e^{-\beta E_j} + \sum_{\text{pairs}} (e^{-\beta E_k} + e^{-\beta E_j^*}) \quad (6)$$

which is real but not necessarily positive. As a consequence of the Bender-Mannheim theorem, we have the following characterization of partition functions: Models which are Hermitian, or equivalent to Hermitian models under a similarity transform, have  $Z$  real and positive for all real  $\beta$ ; models which have generalized  $\mathcal{PT}$  symmetry have  $Z$  real, but not necessarily positive, for all real  $\beta$ . A Laplace transform argument shows that the converse is also true. Thus models with generalized  $\mathcal{PT}$  symmetry are precisely the class of models in which the complex weight problem can be reduced a genuine sign problem, the problem of averaging over positive and negative weights.

#### D. Equivalence to Hermitian if $\mathcal{PT}$ symmetry is unbroken

The difficulty presented by the sign problem depends directly on  $\mathcal{PT}$  symmetry breaking or its absence. Mostafazadeh [30] has proven that when  $\mathcal{PT}$  symmetry is unbroken (region I) and the spectrum is non-degenerate, there is a similarity transformation  $S$  that transforms a  $\mathcal{PT}$ -symmetric Hamiltonian  $H$  into an isospectral Hermitian Hamiltonian  $H_h$  via  $H_h = SHS^{-1}$ . If  $S$  can be found, the transformation of  $H$  into  $H_h$  eliminates the sign problem for  $\mathcal{PT}$ -symmetric quantum Hamiltonians throughout the interior of region I. On the boundary of region I, where two or more eigenvalues become degenerate, it is possible that the Hamiltonian can be of a non-diagonalizable Jordan block form [9]. The equivalence to a Hermitian Hamiltonian also applies to  $\mathcal{PT}$ -symmetric transfer matrices  $T$ , but a further restriction to positive eigenvalues for  $T$  is necessary for the elimination of the sign problem. Thus there are regions of parameter space where the sign problem can be removed by a similarity transformation. Unfortunately, the explicit construction of the similarity transform typically requires knowledge of the exact eigenvalues and eigenvectors. However, there are some models, notably the  $-\lambda x^4$  model, for which the similarity transform or an equivalent functional integral transformation is known [2, 7, 25, 35]. In regions II and III, the sign problem has an underlying physical basis, and cannot be removed by a similarity transformation. The negative weight contributions to the partition function  $Z$  arise from the

contributions of complex conjugate eigenvalue pairs associated with  $\mathcal{PT}$  symmetry breaking. It is that breaking that in turn gives rise to the oscillatory and damped oscillatory behavior of two-point functions characteristic of many physical systems.

### E. Real Representations of $\mathcal{PT}$ -symmetric Hamiltonians

There are  $\mathcal{PT}$  symmetric models like the ANNNI model [39] where the classical Hamiltonian, corresponding to the action in the path integral formalism, is real. Such a model can be simulated with no difficulties of principle throughout its parameter space. In Hermitian systems, the existence of an antiunitary involution commuting with the Hamiltonian implies that there is a basis in which  $H$  is real; see, *e.g.*, [22]. This theorem easily extends to the case of those  $\mathcal{PT}$ -symmetric systems for which  $(\mathcal{PT})^2 = 1$ , and can be applied to transfer matrices as well as Hamiltonians. This suggests the existence of a class of  $\mathcal{PT}$ -symmetric models which can be simulated in all three regions, but no general criterion for determining the class is known.

The proof that for any  $\mathcal{PT}$ -symmetric Hamiltonian there is a basis in which the matrix elements of  $H$  are real follows closely the proof for Hermitian systems [22]. The antiunitary operator  $\mathcal{PT}$  commutes with the Hamiltonian  $[\mathcal{PT}, H] = 0$  and satisfies  $(\mathcal{PT})^2 = 1$ . These properties are sufficient to construct a real representation of the Hamiltonian  $H$ . The first step is the construction of a  $\mathcal{PT}$ -invariant basis  $\psi_a$ . We start from any non-zero vector  $\phi_1$  and complex number  $\alpha_1$ . The vector  $\psi_1 = \alpha_1\phi_1 + \mathcal{PT}\alpha_1\phi_1$  is invariant under  $\mathcal{PT}$ . Choosing a vector  $\phi_2$  orthogonal to  $\psi_1$ , we form the vector  $\psi_2 = \alpha_2\phi_2 + \mathcal{PT}\alpha_2\phi_2$ , where  $\alpha_2$ . The inner product of  $\psi_2$  and  $\psi_1$  is zero:

$$\langle\psi_2|\psi_1\rangle = \alpha_2^* \langle\phi_2|\psi_1\rangle + \alpha_2 \langle\mathcal{PT}\phi_2|\psi_1\rangle = \alpha_2^* \langle(\mathcal{PT})^2\phi_2|\psi_1\rangle + \alpha_2 \langle\mathcal{PT}\psi_2|\psi_1\rangle \quad (7)$$

$$\begin{aligned} \langle\psi_2|\psi_1\rangle &= \alpha_2^* \langle\phi_2|\psi_1\rangle + \alpha_2 \langle\mathcal{PT}\phi_2|\psi_1\rangle \\ &= 0 + \alpha_2 \langle(\mathcal{PT})^2\phi_2|\mathcal{PT}\psi_1\rangle^* \\ &= \alpha_2 \langle\phi_2|\psi_1\rangle^* = 0 \end{aligned}$$

The complex number  $\alpha_2$  can be adjusted to ensure that  $\psi_2$  is not the zero vector. By proceeding in this fashion, a  $\mathcal{PT}$ -symmetric orthogonal basis can be constructed. In this



basis, the matrix elements of the Hamiltonian are real:

$$\begin{aligned}
H_{ab} &= \langle \psi_a | H \psi_b \rangle \\
&= \langle \mathcal{PT} \psi_a | \mathcal{PT} H \psi_b \rangle^* \\
&= \langle \mathcal{PT} \psi_a | H (\mathcal{PT}) \psi_b \rangle^* \\
&= \langle \psi_a | H \psi_b \rangle^* \\
&= H_{ab}^*
\end{aligned}$$

Note that this results holds independent of the appearance of complex eigenvalues in  $H$ . Because  $H$  has only real matrix elements in this basis, it is clear that the secular  $\det(z - H) = 0$  of such a system has only real coefficients, a fact closely linked to  $\mathcal{PT}$  symmetry by the Bender-Mannheim theorem.

### III. SPECTRAL PROPERTIES OF $\mathcal{PT}$ -SYMMETRIC MODELS

Spectral positivity plays a fundamental role in Hermitian systems. As we have seen, it ensures that the partition function  $Z$  is always positive, and it gives a representation of two-point functions as sums of decaying exponentials. On a practical level, it allows for the isolation of the lightest state in a given channel from the large-distance behavior of two-point functions. Because  $\mathcal{PT}$ -symmetric models lead naturally to two different basis sets, completeness and the subsequent derivation of the Kallen-Lehmann representation for two-point functions is more complicated than in the Hermitian case. We give a self-contained derivation of both below, followed by a brief discussion of the implications of our results. Of particular interest is the connection of broken  $\mathcal{PT}$  symmetry of the ground state (region III), with generalized Yang-Lee phase transitions. For simplicity, we will use  $H$  and  $\beta$  throughout this section, but we note that in classical statistical mechanics problems, the relevant objects are  $T$  and  $L$ , in which case  $\beta$  is not the inverse temperature of the system and correlation functions are between different spatial locations. As we will see for two-dimensional QCD in section V, a transfer matrix approach can also be useful for quantum systems as well.

### A. Completeness and Kallen-Lehman representation for $\mathcal{PT}$ -symmetric systems

We now prove a completeness relation for  $\mathcal{PT}$ -symmetric models which is valid in all three regions. We consider the typical case where the Hamiltonian  $H$  is diagonalizable via a similarity transformation and has discrete, non-degenerate eigenvalues. Exceptional points, in the sense of degenerate real eigenvalues, occur at the boundary of region I as well as inside region II and III. There are well-known difficulties in the spectral resolution at these points; see [3] and [9] for specific examples as well as the general discussion in [10]. The passage from region I to region III, where the ground state eigenvalue becomes degenerate, is a critical point analogous to those found in Hermitian models; the best-known example is the Yang-Lee singularity. In analogy with symmetry-breaking behavior in Hermitian models, it is likely necessary to define the behavior at such a point using either an infinitesimal symmetry-breaking perturbation or symmetry-breaking boundary conditions. At this stage of our understanding of  $\mathcal{PT}$ -symmetric models in statistical mechanics, we cannot provide a general prescription, but must handle each model on a case-by-case basis. The case of non-degenerate eigenvalues, in contrast, is tractable for all models. By virtue of the secular equation for the eigenvalues,  $H$  and  $H^T$  are isospectral: the existence of an eigenvalue-eigenvector pair for  $H$

$$H |j\rangle = E_j |j\rangle \quad (8)$$

implies the existence of a corresponding pair for  $H^T$ :

$$H^T |\tilde{j}\rangle = E_j |\tilde{j}\rangle. \quad (9)$$

From the commutation relation  $[H, \mathcal{PT}] = 0$ , we have

$$H\mathcal{P} |\mathcal{T}j\rangle = H\mathcal{PT} |j\rangle = \mathcal{P}TH |j\rangle = \mathcal{P}TE_j |j\rangle = E_j^* \mathcal{P} |\mathcal{T}j\rangle \quad (10)$$

and its Hermitian conjugate

$$\langle \mathcal{T}j | \mathcal{P} H^\dagger = E_j \langle \mathcal{T}j | \mathcal{P}. \quad (11)$$

Noting that  $\mathcal{P}H\mathcal{P} = H^*$  we have

$$\langle \mathcal{T}j | \mathcal{P} H^\dagger = \langle \mathcal{T}j | \mathcal{P} (\mathcal{P}H\mathcal{P})^T = \langle \mathcal{T}j | H^T \mathcal{P} \quad (12)$$

so that we find after multiplying by  $\mathcal{P}$  on the right that

$$\langle \mathcal{T}j | H^T = E_j \langle \mathcal{T}j | \quad (13)$$

Now consider the matrix element

$$\langle \mathcal{T}j | (H^T - H^T) | \tilde{k} \rangle = (E_j - E_k) \langle \mathcal{T}j | \tilde{k} \rangle = 0 \quad (14)$$

The set of eigenstates  $\{|j\rangle\}$  and  $\{|\tilde{k}\rangle\}$  are both complete so we must have

$$\langle \mathcal{T}j | \tilde{k} \rangle \propto \delta_{jk} \quad (15)$$

and also

$$\langle \mathcal{T}\tilde{k} | j \rangle \propto \delta_{jk} \quad (16)$$

Thus we have two completeness relations

$$\sum_j \frac{|j\rangle \langle \mathcal{T}j|}{\langle \mathcal{T}j | j \rangle} = 1 \quad (17)$$

and

$$\sum_j \frac{|\tilde{j}\rangle \langle \mathcal{T}j|}{\langle \mathcal{T}j | \tilde{j} \rangle} = 1. \quad (18)$$

These completeness relations assume the Hamiltonian  $H$  acts in a space in which the inner products  $\langle n | \mathcal{T} \tilde{n} \rangle$  are finite. The consequences of this assumption can vary from model to model. See [6] for a specific example where the contour along which a  $\mathcal{PT}$ -symmetric differential equation is evaluated is deformed into the complex plane to ensure finite inner products. However, this technical point will not be of concern for the models we analyze in this paper. We will generally choose the normalization of states such that  $\langle \mathcal{T} \tilde{j} | j \rangle = \langle \mathcal{T} j | \tilde{j} \rangle = 1$ .

With completeness relations at hand we can now calculate the partition function and spatial two-point functions in terms of eigenvalues and eigenstates. For a quantum theory, the partition function  $Z$  is given by

$$Z = \sum_n \langle n | e^{-\beta H_{PT}} | n \rangle \quad (19)$$

where  $\{|n\rangle\}$  is an arbitrary orthonormal basis; note that the basis formed by the eigenstates of  $H_{PT}$  cannot be used in this way to define  $Z$  unless  $H_{PT}$  is Hermitian. When  $H$  is not Hermitian and  $\mathcal{PT}$  symmetry is unbroken, it is a common practice to require  $\mathcal{PT} |j\rangle = |j\rangle$  and to introduce an additional linear operator  $\mathcal{C}$  such that  $\mathcal{CPT} |j\rangle \cdot |k\rangle = \delta_{jk}$  [4, 5]. Using these conventions, one can write the partition function as a sum over eigenstates of the

form  $Z = \sum_j \langle j | V e^{-\beta H} | j \rangle$  where  $V = (\mathcal{CP})^T$ . The need for the operator  $V$  arises because the eigenstates  $|j\rangle$  are not orthonormal with respect to the inner product  $\langle m | n \rangle$ . However, if  $H$  breaks  $\mathcal{PT}$ -symmetry, not all of the eigenstates of  $H$  are eigenstates of  $\mathcal{PT}$ , and an alternative expression for  $V$  of the form  $V = \sum_j |\mathcal{T}\tilde{j}\rangle \langle \mathcal{T}\tilde{j}|$  would need to be used. We avoid these considerations in this paper by performing the trace in the partition function over an arbitrary orthonormal basis; such a basis may be constructed from the eigenstates  $|j\rangle$  using the Gram-Schmidt algorithm.

We insert the  $\mathcal{PT}$  completeness relation

$$Z = \sum_n \langle n | e^{-\beta H} \sum_j \frac{|j\rangle \langle \mathcal{T}\tilde{j}|}{\langle \mathcal{T}\tilde{j} | j \rangle} | n \rangle = \sum_j e^{-\beta E_j} \frac{\sum_n \langle n | j \rangle \langle \mathcal{T}\tilde{j} | n \rangle}{\langle \mathcal{T}\tilde{j} | j \rangle} = \sum_j e^{-\beta E_j} \quad (20)$$

so that  $Z$  has the same form as in Hermitian theories, as assumed in section II. We can write  $Z$  usefully as

$$Z = \sum_r e^{-\beta E_r} + \sum_p (e^{-\beta E_p} + e^{-\beta E_p^*}) \quad (21)$$

where the sum over  $r$  is over all real energies  $E_r$  and the sum over  $p$  is over pairs of complex energies. The oscillatory character of the second sum leads to negative contributions to the partition function, which is the sign problem. Note that in region I, there is no sign problem. The sign problem only arises in region II and III. Strictly speaking, the sign problem disappears in region II in the limit  $\beta \rightarrow \infty$ . For transfer matrix problems, this implies that in the limit  $L \rightarrow \infty$ , the sign problem becomes negligible in region II. Only in region III does the sign problem survive the infinite volume limit in the calculation of  $Z$ .

## B. Spectral theorems

We now prove some general results for the typical case where  $H$  is symmetric but complex. When  $H$  is symmetric, we have  $|j\rangle = |\tilde{j}\rangle$  and  $|\mathcal{T}j\rangle = |\mathcal{T}\tilde{j}\rangle$  and we immediately obtain the somewhat simpler completeness relation

$$\sum_j |j\rangle \langle \mathcal{T}j| = 1 \quad (22)$$

In typical  $\mathcal{PT}$ -symmetric quantum mechanics models,  $H$  is symmetric, and the completeness relation takes the form [4, 5]

$$\sum_j \frac{\psi_j(x) \psi_j(y)}{\int dx \psi_j^2(x)} = \delta(x - y) \quad (23)$$

showing the explicit normalization factor.

We begin by proving a result for certain matrix elements that appear repeatedly in these calculations. If  $E_j \neq E_j^*$ , then the properly normalized eigenstate of  $H$  with eigenvalue  $E_j^*$  is related to  $\mathcal{PT}|j\rangle$  by a phase factor:

$$\mathcal{PT}|j\rangle = e^{i\alpha_j}|j^*\rangle. \quad (24)$$

It immediately follows that

$$\mathcal{PT}|j^*\rangle = \mathcal{PT}e^{-i\alpha_j}\mathcal{PT}|j\rangle = e^{i\alpha_j}|j\rangle, \quad (25)$$

or

$$e^{i\alpha_{j^*}} = e^{i\alpha_j}. \quad (26)$$

On the other hand, if  $E_j$  is real, we have simply

$$\mathcal{PT}|j\rangle = e^{i\alpha_j}|j\rangle. \quad (27)$$

so in this case we may identify  $|j^*\rangle$  with  $|j\rangle$ . We will prove results for matrix elements in the case where  $E_j$  is complex, and similar results will hold when  $E_j$  is real with  $|j^*\rangle$  replaced by  $|j\rangle$ .

Consider the action of the bra

$$\langle \mathcal{T}j^* | \mathcal{PT} \quad (28)$$

on an arbitrary ket

$$|\psi\rangle = \sum_{pairs} (\chi_k |k_c\rangle + \chi_{k^*} |k_c^*\rangle) + \sum_{reals} \rho_n |n_r\rangle. \quad (29)$$

We have

$$\langle \mathcal{T}j^* | \mathcal{PT} |\psi\rangle = \langle \mathcal{T}j^* | \mathcal{PT} \left[ \sum_{pairs} (\chi_k |k_c\rangle + \chi_{k^*} |k_c^*\rangle) + \sum_{reals} \rho_n |n_r\rangle \right], \quad (30)$$

$$\langle \mathcal{T}j^* | \mathcal{PT} |\psi\rangle = \langle \mathcal{T}j^* | \left[ \sum_{pairs} (\chi_k^* e^{i\alpha_k} |k_c^*\rangle + \chi_{k^*}^* e^{i\alpha_k} |k_c\rangle) + \sum_{reals} \rho_n^* e^{i\alpha_n} |n_r\rangle \right], \quad (31)$$

$$\langle \mathcal{T} j^* | \mathcal{PT} | \psi \rangle = e^{i\alpha_j} \chi_j^*, \quad (32)$$

and

$$\langle \mathcal{T} j^* | \mathcal{PT} | \psi \rangle = e^{i\alpha_j} \langle T j | \psi \rangle^*. \quad (33)$$

Now we apply the above result to a state of the form  $\phi |j^*\rangle$  where  $\mathcal{PT}\phi\mathcal{PT} = \phi$ :

$$\langle \mathcal{T} k^* | \phi_1 | j^* \rangle = \langle \mathcal{T} k^* | PT \phi_1 PT | j^* \rangle \quad (34)$$

$$\langle \mathcal{T} k^* | \phi_1 | j^* \rangle = \langle \mathcal{T} k^* | PT \phi_1 e^{i\alpha_j} | j \rangle \quad (35)$$

$$\langle \mathcal{T} k^* | \phi_1 | j^* \rangle = e^{i\alpha_j} \langle \mathcal{T} k | \phi_1 e^{i\alpha_j} | j \rangle^* \quad (36)$$

$$\langle \mathcal{T} k^* | \phi_1 | j^* \rangle = \langle \mathcal{T} k | \phi_1 | j \rangle^* \quad (37)$$

This result has been proven for the case where both  $|j\rangle$  and  $|k\rangle$  are half of a conjugate pair of eigenvectors. It also holds when one or both of the eigenvectors has a real eigenvalue, in which case we identify  $|j^*\rangle$  with  $|j\rangle$ . In the case where both  $E_j$  and  $E_k$  are real, the matrix element is real:

$$\langle \mathcal{T} k | \phi_1 | j \rangle = \langle \mathcal{T} k | \phi_1 | j \rangle^*. \quad (38)$$

With these results in hand, we now turn to one- and two-point functions in the case that  $H$  is symmetric and fields satisfy  $\mathcal{PT}\phi\mathcal{PT} = \phi$ . We remind the reader again that in application to classical statistical mechanics, the Hamiltonian is related to the transfer matrix by  $T = \exp(-H)$ , and  $\beta$  is identified with the length  $L$  of the system. A one-point function can be written as

$$\begin{aligned} \langle \phi(x) \rangle &= \frac{1}{Z} \text{Tr} [e^{-rH_{PT}} \phi e^{-(\beta-r)H_{PT}}] \\ &= \frac{1}{Z} \sum_{jk} \langle \mathcal{T} j | e^{-rH_{PT}} | k \rangle \langle \mathcal{T} k | \phi e^{-(\beta-r)H_{PT}} | j \rangle \\ &= \frac{1}{Z} \sum_{jk} \langle \mathcal{T} j | e^{-rE_k} | k \rangle \langle \mathcal{T} k | \phi e^{-(\beta-r)E_j} | j \rangle \\ &= \frac{1}{Z} \sum_j e^{-\beta E_j} \langle \mathcal{T} j | \phi | j \rangle \\ &= \frac{1}{Z} \left[ \sum_{\text{pairs}} (e^{-\beta E_j} \langle \mathcal{T} j | \phi | j \rangle + e^{-\beta E_j^*} \langle \mathcal{T} j^* | \phi | j^* \rangle) + \sum_{\text{reals}} e^{-\beta E_j} \langle \mathcal{T} j | \phi | j \rangle \right] \end{aligned} \quad (39)$$

where we have used  $r$  to label the coordinate of  $x$  in the direction along which  $H$  acts. This expression for  $\langle \phi(x) \rangle$  is manifestly real as a consequence of our results for matrix elements.

Similarly, suppose  $x$  and  $y$  are two points separated by a distance  $r$  in the direction in which  $H$  acts. Then the two point function for operator  $\phi_1(x)$  and  $\phi_2(y)$  is defined by

$$\begin{aligned} \langle \phi_1(x) \phi_2(y) \rangle &= \frac{1}{Z} \text{Tr} [\phi_1 e^{-rH_{PT}} \phi_2 e^{-(\beta-r)H_{PT}}] \\ &= \frac{1}{Z} \sum_{jk} e^{-rE_j} e^{-(\beta-r)E_k} \langle \mathcal{T}k | \phi_1 | j \rangle \langle \mathcal{T}j | \phi_2 | k \rangle \end{aligned} \quad (40)$$

which is real using the same reasoning that was applied to the one-point function. This representation establishes the fundamental observable distinction between regions I, II and III. Each term in the spectral representation of the two-point function depends on  $r$  as  $\exp[(E_k - E_j)r]$ . In regions I and II, the ground state is unique, and the terms with  $k = 0$  dominate for large  $\beta$ . In region I, this leads to monotonic exponential decay. In region II, some of the excited states have complex energies, leading to modulated exponential decay in two-point functions.

In region III, the ground state, defined as the state with the lowest value of  $\text{Re}(E)$ , is no longer unique. The states  $|0\rangle$  and  $|0^*\rangle$  will dominate in both  $Z$  and in two-point functions in the limit  $\beta \rightarrow \infty$ , or in the limit  $L \rightarrow \infty$  for transfer matrices. We can take  $\beta$  sufficiently large that all states except  $E_0$  and  $E_0^*$  can be neglected, in which case  $Z$  can be approximated by

$$Z \simeq e^{-\beta E_0} + e^{-\beta E_0^*} \quad (41)$$

and the approximate zeros of the partition function will occur at

$$\text{Im}(E_0) = \frac{(2p+1)\pi}{2\beta} \quad (42)$$

where  $p$  is any integer. This is consistent with a general theory of partition function zeros that can be applied to models with  $\mathcal{PT}$ -symmetric transfer matrices [11]. Under some technical conditions, the partition function in a periodic volume  $V = L^d$  can be written as

$$Z = \sum_m e^{-\beta V f_m} + \mathcal{O}(e^{-L/L_0} e^{-\beta V f}) \quad (43)$$

where  $f = \min_m \text{Re}[f_m]$  and  $L_0$  is of the order of the largest correlation length of the system. The  $f_m$ 's have the interpretation of complex free energy densities, and are independent of  $L$ .

These phases are stable if  $Re(f_m) = f$  or metastable otherwise. The zeros of the partition function are within  $\mathcal{O}(e^{-L/L_0})$  of the solutions of the equations.

$$\begin{aligned} Re(f_m) &= Re(f_n) = f \\ Im(f_m) &= Im(f_n) + (2p+1) \frac{\pi}{\beta V} \end{aligned}$$

for some  $m \neq n$  and  $p \in \mathbb{Z}$ . We can apply this directly to region III, using the representation

$$Z = \sum_{\text{reals}} e^{-LE_r} + \sum_{\text{pairs}} (e^{-LE_p} + e^{-LE_p^*}) \quad (44)$$

of the partition function where we identify  $\beta$  with  $L$ . We identify  $LE_0$  and  $LE_0^*$  as  $\beta L^d f_0$  and  $\beta L^d f_0^*$ , so that the partition function has a zero for values of the parameters such that

$$\beta Im[f_0] = \frac{(2p+1)\pi}{2V} \quad (45)$$

This tells us that the zeros of the partition function lie on the boundary of region III, defined by  $Im[f_0] = 0$ , in the limit  $V \rightarrow \infty$ . As the volume of the system is taken to infinity, the zeros of the partition function lie asymptotically on the boundary between phases. Note that this analysis depends on  $L_0$  remaining finite. At a 2nd-order transition,  $L_0$  goes to infinity and the approximation is invalid. Zeros of  $Z$  in region III can lead to potentially rapid oscillation of  $n$ -point functions, and correlation functions are ill-behaved in the vicinity of such points.

#### IV. $\mathcal{PT}$ SYMMETRY IN CLASSICAL STATISTICAL MECHANICS

In this section we consider several models of classical statistical mechanics that are  $\mathcal{PT}$ -symmetric. In all of these, it is convenient to discuss the one-dimensional version of the model, which is analytically tractable. In addition to models where the classical Hamiltonian, and hence the transfer matrix, is complex, there are also models where the classical Hamiltonian and transfer matrix are real, but the transfer matrix is not symmetric. Such models have a “hidden”  $\mathcal{PT}$  symmetry. In those cases where the classical Hamiltonian is real, the matrix elements of  $T$  are positive. The Perron-Frobenius theorem applies, and the eigenvalue of  $T$  of greatest magnitude will be real. Such models thus may lie in region I or II, but never in region III.



### A. $Z(N)$ Models

$Z(N)$  spin systems with complex magnetic fields arise naturally as simplified models of  $SU(N)$  gauge theories non-zero chemical potential [16], with the case  $N = 3$  corresponding to QCD at finite baryon density. These models are naturally  $\mathcal{PT}$ -symmetric. In these models, there is a clear connection of  $\mathcal{PT}$  symmetry with  $Z(N)$  Fourier transforms. This is not surprising: The Fourier transform of a real function  $f(x)$  on  $R$  obeys

$$\tilde{f}(k)^* = \tilde{f}(-k) \quad (46)$$

or equivalently

$$\tilde{f}(-k)^* = \tilde{f}(k) \quad (47)$$

which is precisely the statement of  $\mathcal{PT}$  symmetry. In spin models with complex weights based on groups such as  $U(1)$ ,  $Z(N)$  and  $SU(N)$ ,  $\mathcal{PT}$  symmetry implies that the character expansion of a  $\mathcal{PT}$ -symmetric model has real coefficients. This explains why the flux-tube model [37, 38] gives a purely real representation of the same physics of the  $Z(3)$  model to which it is dual.  $\mathcal{PT}$  symmetry plays a similar role in the worldline approach to lattice field theories at non-zero chemical potential [14].

On each lattice site  $j$  of a  $Z(N)$  spin model there is a spin  $w_j$ , an element of the group  $Z(N)$  which may be parametrized as  $w_j = \exp(2\pi i n_j / N)$  with  $n_j \in \{0, 1, \dots, N-1\}$  defined modulo  $N$  so that 0 and  $N$  are identified. We take the operator  $\mathcal{P}$  to be charge conjugation, acting as  $n_j \rightarrow -n_j$ , or equivalently  $w_j \rightarrow w_j^*$ . The operator  $\mathcal{T}$  is again complex conjugation. Although  $\mathcal{P}$  and  $\mathcal{T}$  have the same effect on the  $w_j$ 's, one is a linear operator and the other antilinear. We will show below that  $\mathcal{P}$  is implemented as a unitary matrix in the transfer matrix formalism. The classical spin-model Hamiltonian  $H$  is defined by

$$-\beta\mathcal{H} = \sum_{\langle jk \rangle} \frac{J}{2} (w_j w_k^* + w_j^* w_k) + \sum_j [h_R (w_j + w_j^*) + h_I (w_j - w_j^*)] \quad (48)$$

where  $\beta = 1/T$ ,  $J$ ,  $h_R$  and  $h_I$  are real and the sum over  $\langle jk \rangle$  represents a sum over nearest-neighbor pairs.  $H$  is trivially  $\mathcal{PT}$ -symmetric. This class of models has complex Boltzmann weights for  $N \geq 3$  when  $h_I \neq 0$ . In the one-dimensional case, it is convenient to write  $\mathcal{H}$  in the form

$$-\beta\mathcal{H} = \sum_j \left[ \frac{J}{2} (w_j w_{j+1}^* + w_j^* w_{j+1}) + \frac{H_1}{2} (w_j + w_{j+1}) + \frac{H_2}{2} (w_j^* + w_{j+1}^*) \right] \quad (49)$$

where  $H_1$  and  $H_2$  are also real parameters. The partition function is given by the sum over all spin configurations

$$Z = \sum_{\{w_j\}} e^{-\beta\mathcal{H}}. \quad (50)$$

Associated with the Hamiltonian is a transfer matrix such that  $Z = \text{Tr } T^{N_s}$ , where

$$T_{jk} = \exp \left[ \frac{J}{2} (z^j z^{k*} + z^{j*} z^k) + \frac{H_1}{2} (z^j + z^k) + \frac{H_2}{2} (z^{*j} + z^{*k}) \right] \quad (51)$$

and  $N_s$  is the spatial size of the lattice, and  $z = \exp[2\pi i/N]$  is the generator of  $Z(N)$ . The allowed values of  $j$  and  $k$  can be taken to run over either the set  $\{0, 1, \dots, N-1\}$  or the set  $\{1, 2, \dots, N\}$ , and we generally identify the indices 0 and  $N$ .

We define the parity operator  $\mathcal{P}$  by  $\mathcal{P}_{jk} = \delta_{j, N-k}$ , which satisfies  $\mathcal{P}^2 = 1$ . Because  $z^{N-j} = z^{*j}$ , it is easy to see that

$$\mathcal{P}T\mathcal{P} = T^* \quad (52)$$

an equation also satisfied by the Hamiltonian when written in matrix form. This is the fundamental relation of  $\mathcal{PT}$  symmetry, and can also be written as  $[\mathcal{PT}, T] = 0$ .

The discrete Fourier transform, defined by

$$\mathcal{F}_{jk} = \frac{1}{\sqrt{N}} z^{jk}, \quad (53)$$

is a symmetric and unitary operator satisfying  $\mathcal{F}\mathcal{F}^+ = I$ . Furthermore,  $\mathcal{F}^2 = \mathcal{F}^{+2} = \mathcal{P}$ , so we have that the Fourier transform of  $T$ ,  $\tilde{T}$ , obeys

$$\begin{aligned} \tilde{T}^* &= (FTF^+)^* \\ &= F^*T^*F^{+*} \\ &= F^+T^*F \\ &= F^+PTPF \\ &= F^+F^2T(F^+)^2F \\ &= FTF^+ \\ &= \tilde{T} \end{aligned}$$

so we see that the Fourier transform of the transfer matrix is indeed real.

The  $\mathcal{PT}$ -symmetric spin models have a complex order parameter coupled to a complex external field. We can prove that  $\mathcal{PT}$  symmetry implies that the order parameter is real.

Let  $w$  be a spin operator in a  $\mathcal{PT}$ -symmetric  $Z(N)$  spin system. The expectation value of  $w$  is given by

$$\langle w \rangle = \frac{\text{Tr} [w T^{N_s}]}{Z} \quad (54)$$

where  $Z = \text{Tr} [T^{N_s}]$  and  $N_s$  is the extent of the system in the direction in which the transfer matrix  $T$  acts. Using  $\mathcal{PT}$  symmetry, we have

$$\begin{aligned} \langle w \rangle &= \frac{\text{Tr} [P w P^2 T^{N_s} P]}{Z} \\ &= \frac{\text{Tr} [w^* T^{*N_s}]}{Z} \\ &= \langle w \rangle^* \end{aligned}$$

where we have used the fact that  $Z$  is real. The reality of  $\langle w \rangle$  is analogous to the result that  $\langle x \rangle$  is purely imaginary in  $\mathcal{PT}$ -symmetric quantum mechanics. An alternative proof of the reality of  $\langle w \rangle$  can be given: in the representation of the system induced by the discrete Fourier transform, the coefficients of the matrix representations of both  $w$  and  $T$  are all real. Equivalently, this can also be seen easily from the character expansion of expressions like

$$\exp [H_1 z + H_2 z^*] = \sum_{j=0}^{N-1} a_j z^j \quad (55)$$

where all the coefficients  $a_j$  are real if  $H_1$  and  $H_2$  are real.

We illustrate the rich behavior possible in these models using the case of a  $Z(3)$  model in  $d = 1$  [34]. If  $h_I = 0$ , then the transfer matrix  $T$  is Hermitian. When  $h_I \neq 0$ ,  $-\beta H$  is no longer real and  $T$  is no longer Hermitian, but is  $\mathcal{PT}$  symmetric. Figure 1 shows the phase diagram in the  $h_R - h_I$  plane for  $J = 0.2$ . There are four distinct regions. In region Ia, all three eigenvalues of the transfer matrix are real and positive. This region includes the line  $h_I = 0$ , and has properties similar to those found in the Hermitian case. In region Ib, all of the eigenvalues are real, but at least one of them is negative. In region II, the eigenvalue of  $T$  largest in magnitude is real, but the two other eigenvalues form a complex conjugate pair. In region III, the two eigenvalues largest in magnitude form a complex conjugate pair, and the third, smaller, eigenvalue is real. In both region II and region III,  $\mathcal{PT}$  symmetry is broken, but in different ways. Borrowing the terminology from  $\mathcal{PT}$ -symmetric quantum mechanics, we will describe the behavior in region III as  $\mathcal{PT}$ -symmetry breaking of the ground state, while region II is  $\mathcal{PT}$ -symmetry breaking of an excited state. The behavior of the two-point function  $G(|j - k|) = \langle w(j) w^\dagger(k) \rangle$  differs substantially in the three regions. In region I,

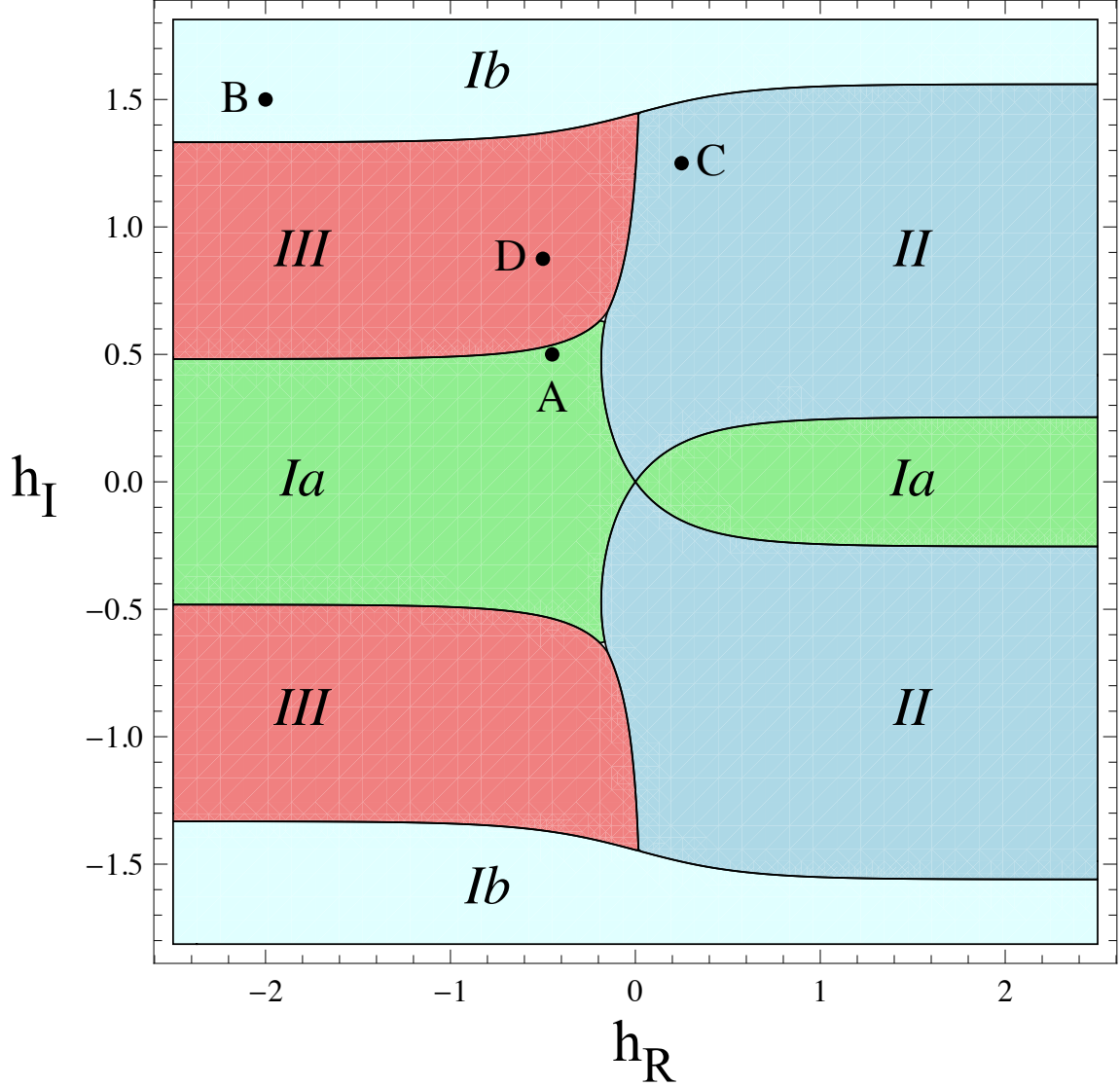


Figure 1: Phase diagram for the  $d = 1$   $\mathcal{PT}$ -symmetric  $Z(3)$  spin model in the  $h_R - h_I$  plane at  $J = 0.2$ . The interpretation of regions Ia, Ib, II and III are given in the text.

the two-point function falls off exponentially. We show typical behavior in region Ia in figure 2 for point A where  $(h_R, h_I) = (-0.45, 0.5)$ . Similar behavior occurs in region Ib, as shown in the figure for point B where  $(h_R, h_I) = (-2.0, 1.5)$ . Although the figure shows that the continuation of the two-point function away from integer values can be negative, note that the values at integer points are all non-negative. The two-point function at point C in region II where  $(h_R, h_I) = (0.25, 1.25)$  shows the damped oscillatory behavior associated with  $\mathcal{PT}$  breaking in excited states. For the point D in region III, where  $(h_R, h_I) = (-0.5, 0.875)$ , the  $\mathcal{PT}$  breaking of the ground state leads to oscillatory behavior of the two-point function in

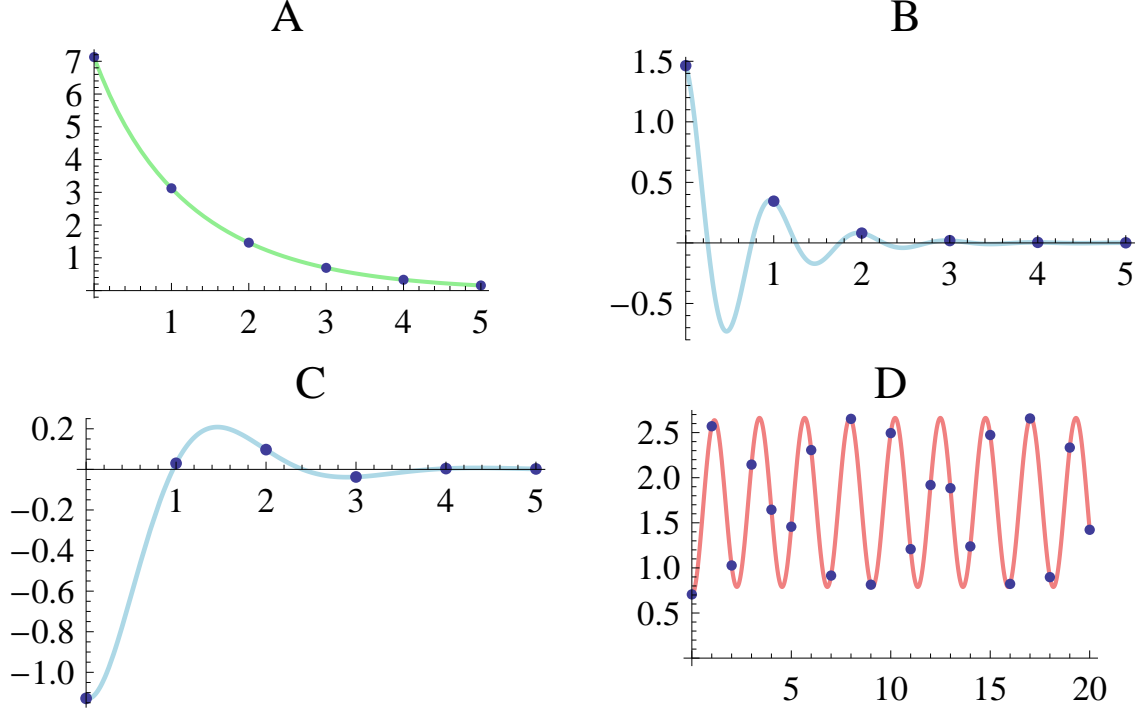


Figure 2: The two-point function as a function of lattice spacing for the parameters corresponding to points A, B, C and D in figure 1.

the limit of large distance. Note that region III only occurs when  $h_R$  is negative. For  $h_R < 0$  and  $h_I = 0$ , the spin configurations with lowest energy have a two-fold degeneracy. With  $h_I = 0$ , the ground state of the transfer matrix is unique. For the case  $h_R < 0$ ,  $h_I = 0$ , and  $J$  large, the splitting of the two lowest eigenvalues of the transfer matrix in  $d = 1$  is small. For sufficiently strong  $h_I$ , the real parts of the two lowest eigenvalues of  $T$  merge, and  $\mathcal{PT}$  symmetry breaking of the ground state occurs.

## B. The chiral Potts model

Our first example of a system with a hidden  $\mathcal{PT}$  symmetry is the chiral Potts model [24, 36]. It is a variant of  $Z(N)$  spin models, and we use the same notation as above. Consider a  $d = 1$   $Z(N)$  spin model with Hamiltonian  $\mathcal{H}$  of the form

$$-\beta\mathcal{H} = \sum_j \left[ \frac{J}{2} (w_j u w_{j+1}^* + w_j^* u^* w_{j+1}) \right] \quad (56)$$

where  $u = \exp(2\pi i \Delta / N)$  with  $\Delta \in [0, 1]$ . The classical Hamiltonian  $\mathcal{H}$  is real, and the model is invariant under the action of  $\mathcal{T}$ , regarded as complex conjugation. However, the

transfer matrix is not Hermitian for general  $\Delta$ . The transfer matrix is given by

$$T_{jk} = \exp \left[ \frac{J}{2} (z^j u z^{k*} + z^{j*} u^* z^k) \right] \quad (57)$$

where as before  $z = \exp(2\pi i/N)$ . The reality of  $\mathcal{H}$  implies that  $T_{jk}^* = T_{jk}$ , and thus possesses a generalized  $\mathcal{PT}$  symmetry, with  $\mathcal{P}$  simply taken to be the identity. Although  $T$  is real, it is not symmetric in general, because  $T^T \neq T$ . Because the transfer matrix has only real positive entries, by the Perron-Frobenius theorem the correlation functions of the chiral Potts model can exhibit region I or region II behavior, but never region III.

(58)

### C. The ANNNI model

The Anisotropic Next-Nearest-Neighbor Ising (ANNNI) model [39] is a prototypical example of a system that appears as if it “should” have a Hermitian transfer matrix, but does not. Instead, the model has a generalized  $\mathcal{PT}$  symmetry which underlies the model’s unusual phase structure [34]. The one-dimensional model is exactly solvable, and has a reduced Hamiltonian

$$\beta H = -K_1 \sum_j s_j s_{j+1} - K_2 \sum_j s_j s_{j+2} \quad (59)$$

where  $K_1$  and  $K_2$  are real couplings and the Ising spins take on the values  $\pm 1$ . The Hamiltonian is real, and stochastic simulations of the model may be carried out with ease. One approach to solving the model is to construct a  $4 \times 4$  transfer matrix between nearest neighbor pairs

$$T_4 = \begin{pmatrix} e^{2K_1+2K_2} & e^{K_1} & e^{-K_1} & e^{-2K_2} \\ e^{-K_1} & e^{2K_2-2K_1} & e^{-2K_2} & e^{K_1} \\ e^{K_1} & e^{-2K_2} & e^{2K_2-2K_1} & e^{-K_1} \\ e^{-2K_2} & e^{-K_1} & e^{K_1} & e^{2K_1+2K_2} \end{pmatrix} \quad (60)$$

The partition function for  $N$  spins, with  $N$  even and periodic boundary conditions, is given by  $Z = \text{Tr} [T_4^{N/2}]$ . The matrix  $T_4$  is real but not symmetric. It commutes with a generalized

parity operator  $\mathcal{P}$  of the form

$$\mathcal{P} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad (61)$$

which implements the symmetry of the model under  $s \rightarrow -s$ ;  $\mathcal{T}$  is complex conjugation, and acts trivially on  $T_4$ . The combination of the reality of  $T_4$  together with  $[T_4, P] = 0$  establishes that  $T_4$  is  $\mathcal{PT}$ -symmetric. There is another approach to solving the one-dimensional model which better displays its  $\mathcal{PT}$  symmetry. We introduce a set of bond variables  $\sigma_j$  into the partition function  $Z$  which we force to be equal to  $s_j s_{j+1}$  via the  $Z_2$  delta function  $(1 + \sigma_j s_j s_{j+1})/2$ . We can then write  $s_j s_{j+2} = \sigma_j \sigma_{j+1}$  in the Hamiltonian. It appears that the new Hamiltonian is simply

$$\beta H = -K_1 \sum_j \sigma_j - K_2 \sum_j \sigma_j \sigma_{j+1} \quad (62)$$

and the model reduces to a standard Ising model in an external field. This is somewhat misleading, because there remains a determinantal factor associated with the change of variables

$$Z = \sum_{\{s\}} \sum_{\{\sigma\}} \prod_j \left[ \frac{1 + \sigma_j s_j s_{j+1}}{2} \right] e^{-\beta H} \quad (63)$$

Carrying out the sum over the  $s$  variables with periodic boundary conditions, we find

$$Z = \sum_{\{\sigma\}} \left[ 1 + \prod_j \sigma_j \right] e^{-\beta H} \quad (64)$$

which tells us that there is a global constraint on the partition function: only configurations with  $\prod_j \sigma_j = 1$  contribute. Let  $T_2$  be the  $2 \times 2$  transfer matrix of the one-dimensional Ising model in an external field

$$T_2 = \begin{pmatrix} e^{K_2+K_1} & e^{-K_2} \\ e^{-K_2} & e^{K_2-K_1} \end{pmatrix}. \quad (65)$$

We define another matrix,  $\tilde{T}_2$ , as

$$\tilde{T}_2 = \sigma_3^{1/2} T_2 \sigma_3^{1/2} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \begin{pmatrix} e^{K_2+K_1} & e^{-K_2} \\ e^{-K_2} & e^{K_2-K_1} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \quad (66)$$

such that the transfer matrix of the model is the  $4 \times 4$  matrix  $\tilde{T}_4 = T_2 \oplus \tilde{T}_2$ . The square of the eigenvalues of  $\tilde{T}_4$  are the eigenvalues of  $T_4$ , as they must be, and  $Z = \text{Tr} [\tilde{T}_4^N]$ . The transfer

matrix  $\tilde{T}_4$  is invariant under  $\mathcal{PT}$ , with the parity operator  $\mathcal{P}$  given by  $1 \oplus \sigma_3$ , and  $\mathcal{T}$  given by complex conjugation. This construction leads directly to the same eigenvalues found in [39]. The eigenvalues of  $T_2$  are of course always real, while the eigenvalues of  $\tilde{T}_2$  are either real or form a conjugate pair. For  $\cosh K_1 > e^{-2K_2}$ , the eigenvalues of  $\tilde{T}_2$  are real, and the spin-spin two-point function decays exponentially. The system is in region I. For  $\cosh K_1 < e^{-2K_2}$ , the eigenvalues of  $\tilde{T}_2$  are complex, and the spin-spin two-point function shows a periodic modulation of its exponential decay. This is region II, and the line  $\cosh K_1 = e^{-2K_2}$  defines the disorder line separating the two regions. The eigenvalues of  $\tilde{T}_2$  are always smaller in absolute value than the eigenvalues of  $T_2$  in this model, so region III does not occur in the  $d = 1$  ANNNI model.

## V. $\mathcal{PT}$ SYMMETRY IN QUANTUM STATISTICAL MECHANICS MODELS

All quantum many-body problems involving a non-zero chemical potential may be described in terms of a non-Hermitian Hamiltonian with generalized  $\mathcal{PT}$  symmetry [34]. At first glance, this is surprising, but it is a simple consequence of the use of Wick rotation and the Euclidean formalism for equilibrium statistical mechanics. This  $\mathcal{PT}$ -symmetric description is closely related to the sign problem. We will explain in detail how the sign problem arises in QCD with heavy quarks at non-zero chemical potential. The two-dimensional case will be solved numerically as an application of  $\mathcal{PT}$  symmetry to this class of problems [33, 34].

### A. $\mathcal{PT}$ symmetry at finite density

We start from a theory with a Hermitian Hamiltonian  $H$  and a conserved global quantum number  $N$ , obtained from a conserved current  $j^\nu$ , that commutes with  $H$ . We assume that  $H$  is Hermitian and invariant under the combined action of time reversal  $\mathcal{T}$  and a charge conjugation  $\mathcal{C}$  that reverses the sign of  $j^\nu$ . We take the number of spatial dimensions to be  $d - 1$ , and the spatial volume to be  $L^{d-1}$ . The grand canonical partition function at temperature  $T = \beta^{-1}$  and chemical potential  $\mu$  is given by  $Z = \text{Tr} [\exp(-\beta H + \beta \mu N)]$ . If  $Z$  is written as a Euclidean path integral, the time component of the current  $j^0$  will Wick rotate to  $ij^d$ , while the chemical potential  $\mu$  does not change. This leads directly to a non-



positive weight in the path integral, and is the origin of the sign problem in finite density calculations. The Euclidean space Lagrangian density may be written as  $\mathcal{L} - i\mu j^d$  where  $\mathcal{L}$  is the Euclidean Lagrangian for  $\mu = 0$ ;  $\mathcal{L} - i\mu j^d$  is complex. The nature of the problem is changed by changing the direction of Euclidean time, so that we are now considering a problem at zero temperature with one compact spatial dimension of circumference  $\beta$ . Upon returning to Minkowski space,  $\mu$  does not rotate. We pick, say, the  $\nu = 1$  direction to be the new time direction and the new inverse temperature is  $L$ . When  $\mu = 0$ , the original Hamiltonian is obtained, but for  $\mu \neq 0$  the partition function is now given by

$$Z = \text{Tr} [e^{-LH_\beta}] \quad (67)$$

where

$$H_\beta = H - i\mu \int d^{d-1}x j^d. \quad (68)$$

The new Hamiltonian  $H_\beta$  is non-Hermitian, but possesses a generalized  $\mathcal{PT}$  symmetry, where the role of  $\mathcal{P}$  is played by the charge conjugation operator  $\mathcal{C}$  that changes the sign of  $j^0$  and  $N$ . Under the combined action of  $\mathcal{CT}$ ,  $j^d \rightarrow -j^d$  and  $i \rightarrow -i$ , leaving the Hamiltonian  $H_{PT}$  invariant. If we introduce the operator  $H_L = H - \mu N$ , we have the relation

$$Z = \text{Tr} [e^{-\beta H_L}] = \text{Tr} [e^{-LH_\beta}] \quad (69)$$

induced by the space-time transformation that exchanges directions 1 and  $d$ . Note that  $Z$  is obtained from  $H_L$  by a sum over all eigenstates, but is dominated by the ground state of  $H_\beta$  in the limit of large  $L$ .

## B. $d = 2$ gauge theories

Within the Euclidean space formalism, a non-zero temperature  $T$  is obtained by making the bosonic fields periodic in Euclidean time, with period  $\beta = 1/T$ . On the other hand, a non-zero chemical potential must be implemented in a way that makes the weight function used in the Feynman path integral complex, as we have seen above. We will show below exactly how QCD with quarks at finite density may be interpreted as a theory with  $\mathcal{PT}$  symmetry.

The Polyakov loop plays a crucial role. Defined as a path-ordered exponential of the

gauge field, in  $3 + 1$  dimensions the Polyakov loop operator  $P$  is given by

$$P(\vec{x}) = \mathbb{P} \exp \left[ i \int_0^\beta dt A_4(\vec{x}, t) \right], \quad (70)$$

and represents the insertion of a static quark into a thermal system of gauge fields at a temperature  $T = \beta^{-1}$ . Figure 3 shows the Polyakov loop in this geometry. Because of the periodic boundary conditions in the Euclidean time direction, the Polyakov loop is a closed loop, and its trace is gauge invariant. Also known as the Wilson line, the Polyakov loop represents the insertion of a static quark at a spatial point  $\vec{x}$  in a gauge theory at finite temperature. In particular, the thermal average of the trace of  $P$  in an irreducible representation  $R$  of the gauge group is associated with the additional free energy  $F_R$  required to insert a static quark in the fundamental representation via

$$\langle \text{Tr}_R P(\vec{x}) \rangle = e^{-\beta F_R}. \quad (71)$$

Pure  $SU(N)$  gauge theories have a global  $Z(N)$  symmetry  $P \rightarrow zP$  where  $z = e^{\frac{2\pi i}{N}}$  is the generator of  $Z(N)$ , the center of  $SU(N)$ . This symmetry, if unbroken, guarantees that for the fundamental representation  $F$ ,  $\langle \text{Tr}_F P(\vec{x}) \rangle = 0$ . This is interpreted as  $F_F$  being infinite, and an infinite free energy is required to insert a heavy quark into the system. On the other hand, if the  $Z(N)$  symmetry is spontaneously broken, the free energy required is finite. Thus confinement in pure gauge theories is associated with unbroken center symmetry, and broken symmetry with a deconfined phase. The Polyakov loop is the order parameter for the deconfinement transition in pure gauge theories  $\langle \text{Tr}_F P \rangle = 0$  in the confined phase and  $\langle \text{Tr}_F P \rangle \neq 0$  in the deconfined phase. The addition of dynamical quarks in the fundamental representation explicitly breaks this  $Z(N)$  symmetry. Nevertheless, the Polyakov loop remains important in describing the behavior of the system, as we will see in our treatment of the sign problem.

In pure gauge theories, the Wilson loop operator is used to measure the string tension between quarks in the confined phase where  $F_R$  vanishes for representations transforming non-trivially under  $Z(N)$ . At non-zero temperature, a timelike string tension  $\sigma_k^{(t)}$  between  $k$  quarks and  $k$  antiquarks can be measured from the behavior of the correlation function

$$\left\langle \text{Tr}_F P^k(\vec{x}) \text{Tr}_F (P^+(\vec{y}))^k \right\rangle \simeq \exp \left[ -\frac{\sigma_k^{(t)}}{T} |\vec{x} - \vec{y}| \right] \quad (72)$$

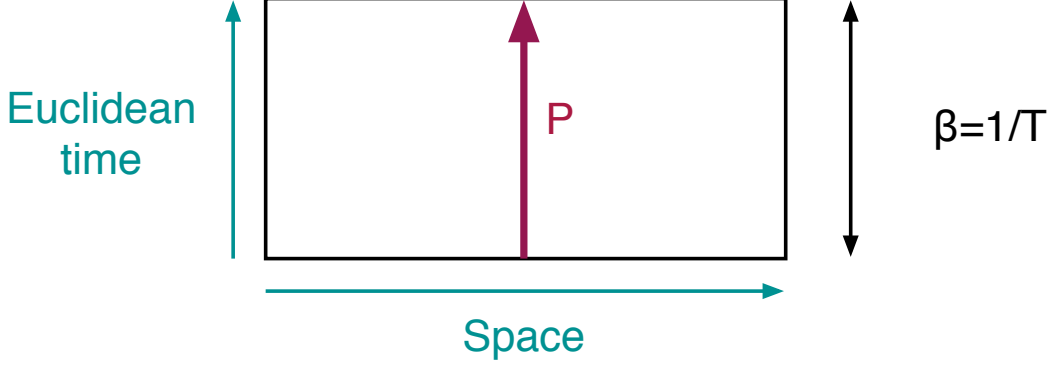


Figure 3: The Polyakov loop in Euclidean space-time.

at sufficiently large distances. A confining phase is defined by two properties: the expectation value  $\langle Tr_R P \rangle$  is zero for all representations  $R$  transforming non-trivially under  $Z(N)$ , and the string tensions  $\sigma_k^{(t)}$  must be non-zero for  $k = 1$  to  $N - 1$ .

Perturbation theory can be used to calculate the one-loop free energy density  $f_q$  of quarks in  $d + 1$  dimensions in the fundamental representation with spin degeneracy  $s$  moving in a Polyakov loop background at non-zero temperature  $T = \beta^{-1}$  and chemical potential  $\mu$

$$f_q = -sT \int \frac{d^d k}{(2\pi)^d} Tr_R [\ln (1 + P e^{\beta\mu - \beta\omega_k}) + \ln (1 + P^+ e^{-\beta\mu - \beta\omega_k})] \quad (73)$$

where  $\omega_k = \sqrt{k^2 + M^2}$  is the energy of the particle as a function of  $k$  and  $M$  is the mass of the particle [21, 42]. The expression for a bosonic field is similar. The logarithm can be expanded to give

$$f_q = sT \int \frac{d^d k}{(2\pi)^d} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} [e^{n\beta\mu - n\beta\omega_k} Tr_R P^n + e^{-n\beta\mu - n\beta\omega_k} Tr_R P^{+n}]. \quad (74)$$

This expression has a simple interpretation as a sum of paths winding around the timelike direction. With standard boundary conditions, which are periodic for bosons and antiperiodic for fermions, this one-loop free energy always favors the deconfined phase.

The effects of heavy quarks in the fundamental representation, with  $\beta M \gg 1$ , on the gauge theory can be obtained approximately from the  $n = 1$  term in the free energy

$$f_q \approx -sT \int \frac{d^d k}{(2\pi)^d} Tr_F [P e^{\beta\mu - \beta\omega_k} + P^+ e^{-\beta\mu - \beta\omega_k}] \quad (75)$$

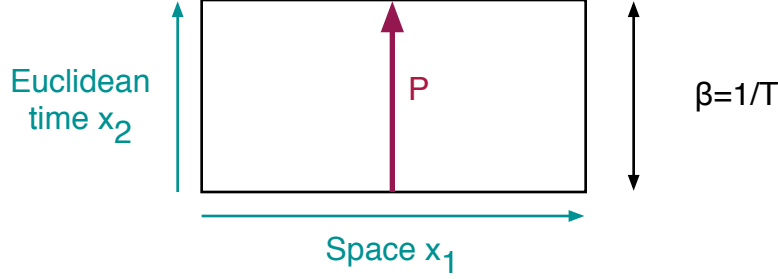


Figure 4: The Polyakov loop in  $(1+1)$ -dimensional space-time.

because term with higher  $n$  are suppressed by a factor  $e^{-n\beta M}$ . In this approximation, bosons and fermions have the same effect at leading order. After integrating over  $k$ , the free energy  $f_q$  can be written as  $f_q \approx -h_F [e^{\beta\mu} \text{Tr}_F P + e^{-\beta\mu} \text{Tr}_F P^+]$ . The one-loop free energy density is the one-loop effective potential at finite temperature. Thus the free energy for the heavy quarks can be added to the usual gauge action to give an effective action which involves only the gauge fields. The effective action is given by

$$S_{eff} = \int d^{d+1}x \left[ \frac{1}{4g^2} (F_{\mu\nu}^a)^2 - h_F (e^{\beta\mu} \text{Tr}_F(P) + e^{-\beta\mu} \text{Tr}_F(P^+)) \right] \quad (76)$$

and the structure and symmetries of the theory are obviously the same in any number of spatial dimensions. Because  $\text{Tr}_F P$  is complex for  $N \geq 3$ , the effective action for the gauge fields is complex. This is a form of the so-called sign problem for gauge theories at finite density: the Euclidean path integral involve complex weights. This problem is a fundamental barrier to lattice simulations of QCD at finite density.

### C. Heavy quarks at $\mu \neq 0$ in two dimensions and $\mathcal{PT}$ symmetry

In one space and one time dimension, the field theory arising from the effective action  $S_{eff}$  can be reduced to a  $\mathcal{PT}$ -symmetric Hamiltonian acting on class functions of the gauge group. The effective action, including the effects of heavy quarks, is

$$S_{eff} = \int d^2x \left[ \frac{1}{4g^2} (F_{\mu\nu}^a)^2 - h_F (e^{\beta\mu} \text{Tr}_F(P) + e^{-\beta\mu} \text{Tr}_F(P^+)) \right] \quad (77)$$

where the gauge field  $A_\mu$  now has two components. Figure 4 shows the Polyakov loop in a  $1+1$ -dimensional geometry. It is convenient to work in a gauge where  $A_1 = 0$ ; this is turn

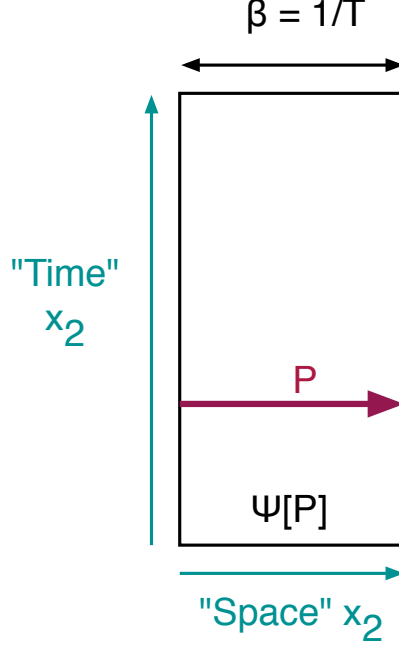


Figure 5: The Polyakov loop in a  $(1 + 1)$ -dimensional transfer matrix geometry.

implies that  $A_2$  depends only on  $x_1$ . After integration over  $x_2$ , we are left with a Lagrangian

$$L = \frac{\beta}{2g^2} \left( \frac{dA_2^a}{dx_1} \right)^2 - h_F \beta \left[ e^{\beta\mu} \text{Tr}_F(P) + e^{-\beta\mu} \text{Tr}_F(P^+) \right] \quad (78)$$

which we regard as the Lagrangian for a system evolving as a function of a time coordinate  $x_1$ . This represents a change from a Euclidean time point of view to a transfer matrix geometry, as shown in figure 5. In this geometry, the Polyakov loop represents the insertion of an electric flux line in a box with periodic boundary conditions, and the free energy density is obtained from the lowest-lying eigenvalue of the transfer matrix.

The physical states of the system are gauge-invariant, meaning that they are class functions of  $P$ :  $\Psi[P] = \Psi[gPg^+]$ . The group characters form an orthonormal basis on the physical Hilbert space:  $\Psi[P] = \sum_R a_R \text{Tr}_R(P)$ . The Hamiltonian  $H$ , obtained from  $L$ , acts on the physical states as

$$H = \frac{g^2\beta}{2} C_2 - h_F \beta \left[ e^{\beta\mu} \text{Tr}_F(P) + e^{-\beta\mu} \text{Tr}_F(P^+) \right] \quad (79)$$

where  $C_2$  is the quadratic Casimir operator for the gauge group, the Laplace-Beltrami operator on the group manifold. We have thus reduced the problem of heavy quarks at finite

density in two dimensions to a problem of quantum mechanics on the gauge group. Unfortunately, the Hamiltonian  $H$  is not Hermitian when  $\mu \neq 0$ , and thus cannot be relied upon to have real eigenvalues. This is a direct manifestation of the sign problem.

Although the Hamiltonian  $H$  is not Hermitian when  $\mu \neq 0$ , it is  $\mathcal{PT}$ -symmetric under the transformations

$$\mathcal{P} : x_2 \rightarrow -x_2 \quad A_2 \rightarrow -A_2 \quad (80)$$

$$\mathcal{T} : i \rightarrow -i \quad (81)$$

which should be regarded as parity and time-reflection in the transfer matrix geometry. Together these lead to

$$\mathcal{PT} : P \rightarrow P \quad (82)$$

which leaves the Hamiltonian invariant. If this  $\mathcal{PT}$ -symmetry is unbroken, the eigenvalues of the Hamiltonian will be real, and there is no sign problem. The  $\mathcal{PT}$  symmetry remains even in the high-density limit where the quark mass  $M$  and chemical potential  $\mu$  are taken to infinity in such a way that antiparticles are suppressed and  $P^+$  does not appear in  $H$ .

The simplest non-trivial gauge group is  $SU(3)$ , because the cases of  $U(1)$  and  $SU(2)$  are atypical. For the gauge group  $U(1)$ , the Hamiltonian  $H$  may be written as

$$H = -\frac{e^2\beta}{2} \frac{d^2}{d\theta^2} - h_F\beta (e^{\beta\mu+i\theta} + e^{-\beta\mu-i\theta}) \quad (83)$$

but a simple change of variable  $\theta \rightarrow \theta + i\beta\mu$  eliminates  $\mu$ :

$$H = -\frac{e^2\beta}{2} \frac{d^2}{d\theta^2} - h_F\beta (e^{+i\theta} + e^{-i\theta}) \quad (84)$$

This is very similar to the case of the two-dimensional  $\mathcal{PT}$ -symmetric sine-Gordon model considered in [8]. In the case of  $SU(2)$ , all the irreducible representations are real, and the Hamiltonian is Hermitian:

$$H_{SU(2)} = \frac{g^2\beta}{2} C_2 - 2h_F \cosh(\beta\mu) \chi_{j=1/2}(P). \quad (85)$$

In general there is no sign problem in  $SU(2)$  gauge theories at finite density holds in general, and this feature has been exploited in lattice simulations with  $\mu \neq 0$  [23, 26].

Thus  $N = 3$  is the first non-trivial case for  $SU(N)$  gauge groups. We have calculated the lowest eigenvalues of  $H$  using finite dimensional approximants. It is convenient to work in

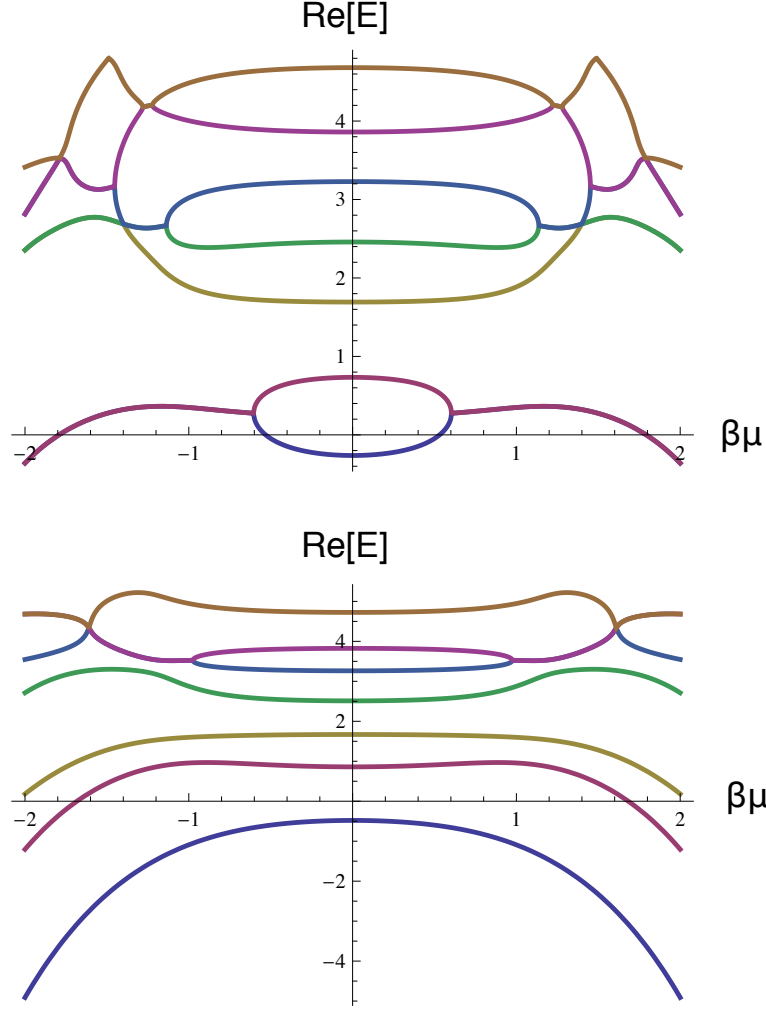


Figure 6: The real part of the  $SU(3)$  Hamiltonian  $H_\beta$  as a function of  $\beta\mu$ . The upper graph is for periodic boundary conditions for the heavy quarks, while the lower graph is for antiperiodic boundary conditions. The energy has been scaled such that  $g^2\beta/2$  is set equal to 1.

the group character basis. The Casimir operator  $C_2$  is diagonal in this basis, and characters act as raising and lowering operators. For example, in the  $4 \times 4$  subspace spanned by the 1, 3,  $\bar{3}$ , and 8 representations of  $SU(3)$ , the Hamiltonian takes the form

$$\begin{pmatrix} 0 & e^{-\beta\mu}h_F\beta & e^{\beta\mu}h_F\beta & 0 \\ e^{\beta\mu}h_F\beta & \frac{4}{3} \cdot \frac{g^2\beta}{2} & e^{-\beta\mu}h_F\beta & e^{\beta\mu}h_F\beta \\ e^{-\beta\mu}h_F\beta & e^{\beta\mu}h_F\beta & \frac{4}{3} \cdot \frac{g^2\beta}{2} & e^{-\beta\mu}h_F\beta \\ 0 & e^{-\beta\mu}h_F\beta & e^{\beta\mu}h_F\beta & 3 \cdot \frac{g^2\beta}{2} \end{pmatrix}. \quad (86)$$

If  $h_F$  is set to zero, we see that the eigenvalues are proportional to Casimir invariants 0,  $4/3$ ,  $4/3$ , and 3 for the 1, 3,  $\bar{3}$ , and 8 representations of  $SU(3)$ . We have therefore removed

an overall factor of  $g^2\beta/2$ , so the overall strength of the potential term is controlled by the dimensionless parameter  $2h_F/g^2$ . The resulting dimensionless energy eigenvalues are thus normalized to give the quadratic Casimir operator when  $2h_F/g^2 = 0$ . The lowest eigenvalues have been calculated numerically using a basis of dimension nine or larger, with the stability of the lowest eigenvalues checked by changing the basis size.

The parameter  $h_F$  is positive for fermions with antiperiodic boundary conditions in the timelike direction, which are required for spectral positivity. However, it is also of interest to consider the case of periodic boundary conditions for the heavy quarks, corresponding to  $h_F < 0$  [31, 32, 41]. In figure 6, we show the real part of the eigenvalues of  $H_\beta$ , measured in units where  $g^2\beta/2$  is set to 1. The overall strength of the potential term is set by the dimensionless parameter  $2h_F/g^2$ . In the upper graph,  $2h_F/g^2 = -0.5$ , corresponding to periodic boundary conditions for the heavy quarks. The lower graph shows the real part of the energy eigenvalues for  $2h_F/g^2 = 0.5$ . In both cases, we see the real parts of pairs of energy eigenvalues coalescing as  $\beta\mu$  is increased. At the point where the real parts become identical, these energy eigenvalues acquire an imaginary part, indicative of broken  $\mathcal{PT}$  symmetry. In the case of periodic boundary conditions, we see that the ground state shows  $\mathcal{PT}$ -symmetry breaking before any of the higher states; thus for large  $\beta\mu$  this places the system in region III. Note that for  $N \geq 3$ , the heavy quark finite density problem of  $SU(N)$  gauge theory is in the universality class of the Lee-Yang problem for  $Z(N)$  spin systems [16]. In the physical case of antiperiodic boundary conditions,  $\mathcal{PT}$ -symmetry breaking appears to occur only in excited states. In the case where all eigenvalues are real, which appears to hold for small  $\beta\mu$ ,  $\mathcal{PT}$ -symmetry is unbroken and the system is in region I. This in turn implies that for small  $\beta\mu$  the sign problem may be solved in principle by a similarity transform to a Hermitian Hamiltonian. For large  $\beta\mu$ , the  $\mathcal{PT}$  symmetry is broken in some of the excited states, which will lead to the region II behavior of sinusoidal decay of spatial correlation functions at high density.

## VI. CONCLUSIONS

For Hermitian systems, there is a well-developed understanding of critical behavior and phase structure, connecting a wide range of systems from simple classical spin systems to exotic quantum field theories. For  $\mathcal{PT}$ -symmetric models, we are in a sense starting over



again with a richer, larger class of systems. There are indications that  $\mathcal{PT}$  symmetry is crucial to the understanding of the sign problem. More generally, the characterization of the phase structure and universality classes of  $\mathcal{PT}$ -symmetric systems is a logical extension of the successful effort to characterize critical phenomena in Hermitian systems.

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